Mapping of sample collection data: GIS tools for the natural product researcher

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Abstract:

Scientists engaged in the research of natural products often either conduct field collections themselves or collaborate with partners who do, such as botanists, mycologists, or SCUBA divers. The information gleaned from such collecting trips (e.g. longitude/latitude coordinates, geography, elevation, and a multitude of other field observations) have provided valuable data to the scientific community (e.g., biodiversity), even if it is tangential to the direct aims of the natural products research, which are often focused on drug discovery and/or chemical ecology. Geographic Information Systems (GIS) have been used to display, manage, and analyze geographic data, including collection sites for natural products. However, to the uninitiated, these tools are often beyond the financial and/or computational means of the natural product scientist. With new, free, and easy-to-use geospatial visualization tools, such as Google Earth, mapping and geographic imaging of sampling data are now within the reach of natural products scientists. The goals of the present study were to develop simple tools that are tailored for the natural products setting, thereby presenting a means to map such information, particularly via open source software like Google Earth.

Keywords: Geographic Information Systems (GIS); Global positioning systems (GPS); OpenGIS® KML Encoding Standard (OGC KML); Geospatial science; Mapping; Google Earth

Article:

1. Introduction

Almost everyone is familiar with the expression – "a picture is worth a thousand words" – the point being that the visualization of something (e.g. data for scientists) is much more vibrant and informative than a written description could ever be. With this axiom in mind, our research team has encountered challenges when describing the strategy behind and the results from our collections of natural product study materials. Even when we went to great lengths to explain verbally and/or in writing why certain collections were interesting or exciting, particularly from rare, extreme, and/or under investigated ecological niches, the points could have been made better with pictures and/or images.

Specifically, we have studied the plant ([Alali et al., 2005], [Alali et al., 2007] and [Alali et al., 2008]) and microbial (Oberlies et al., 2008) biodiversity of the Hashemite Kingdom of Jordan (Jordan) for a number of years. A continual challenge has been to impress upon the scientific community the value of studying ecosystems in this region of the world. We could discuss: the nature preserves across four distinct biogeographic regions (Al-Eisawi, 1998); the confluence of the flora seen in three continents (Feinbrun-Dothan, 1986); the steep change in elevation within relatively compact geopolitical borders; and, even, features that distinguish it from anywhere else in the world, such as the Dead Sea, being 400 m below sea level, the lowest place on terrestrial earth. Yet, it seemed that these arguments were lost on many people. This became evident when a colleague from the United States, making a joke in reference to the sand storms seen in the movie *Lawrence of Arabia*, asked if Jordan was "just a big sandbox." In point of fact, this misconception, that desert environments lack biodiversity, particularly with respect to soil microorganisms, is incorrect (Fierer and Jackson, 2006).

To address this, we began working with experts in Geographic Information Systems (GIS) to develop maps of our collections. This was both for planning purposes, to strategize where to collect samples based on the geographic distribution of many variables (e.g. terrain, precipitation, elevation, soil pH, metals concentrations, and ease of access) and for descriptive purposes, to illustrate pictorially the variety and distinguishing features of the sample points. In other words we wanted to show that the samples were not gathered at random in a “sandbox,” but rather, that they were collected strategically across several ecological niches.
Natural products scientists at Research Triangle Institute (RTI) have access to RTI's staff of GIS professionals to assist with the geospatial data processing, integration, and mapping. However, it is anticipated that most natural products scientists do not have access to professional GIS resources. Therefore, our team has developed a simple conversion program, making use of readily available, powerful visualization tools, such as Google Earth, to facilitate data mapping for the natural products community. Using these tools, we submit that satellite imagery from just four collection sites in Jordan (Fig. 1) illustrates the variety of ecosystems there better than verbose written descriptions.

FIGURE 1 IS OMITTED FROM THIS FORMATTED DOCUMENT

Mapping field collections can be advantageous for the natural products community for a number of reasons. As a short list, mapping facilitates: (1) visualizing the relationship between the sampled locations and other features of the landscape; (2) visualizing the relationship between individual and/or groups of sample sites, particularly over time; (3) examining clustering or dispersion characteristics of data; (4) identifying gaps in sampling locations and planning of future collecting trips; (5) recognition of common data entry errors that are difficult to see when examined in tabular lists (e.g. a data point that lies in an adjacent country due to transposing a number); and (6) communicating and explaining sampling data to others. Moreover, comparing the geographic distribution of scientific data is a growing area of interest that is applicable to many fields. It permits the evaluation of even old data in new ways, and as just one example, a recent paper examined the geographic origins of emerging infectious diseases from 1940 to 2004, showing non-random global patterns (Jones et al., 2008).

As Google Earth (http://earth.google.com) is widely available, free, extremely powerful for mapping and visualization, and likely to only improve over time, we developed a tool to convert natural products sampling data and locations into Google's Keyhole Markup Language (KML), which has been adopted as an open standard by the Open Geospatial Consortium, Inc. (OGC) and is now called OpenGIS®KML Encoding Standard (OGC KML). Google provides high resolution satellite imagery (of varying scales) for the entire globe along with a simple, intuitive interface that requires very little training or experience to learn and that can be run on common desktop computers. The subsequent KML files are readable by Google Earth, permitting the user to quickly generate informative maps of disparate data types (e.g. satellite imagery, roads, terrain, topography). The details for loading and running the software are provided below. This was designed as an open source program to be shared amongst the natural products community. Hopefully, through widespread use and dissemination, its functionality will evolve and improve over time.

2. Results and discussion

The three approaches to enter data into the conversion program (termed ‘csv2kml’), thereby setting the stage for mapping in Google Earth, are outlined in Fig. 2. In all three the entry point into Google Earth is a KML file; therefore, a major goal of this manuscript is to explain how to prepare data for ready conversion into the KML format.

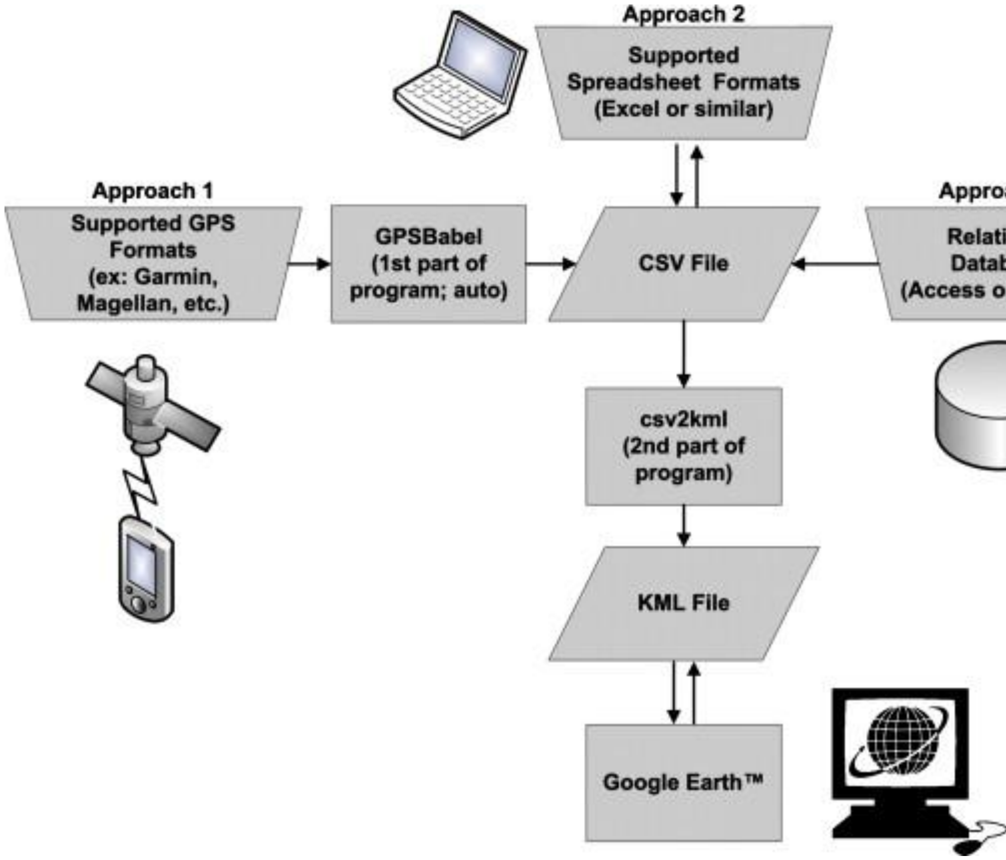


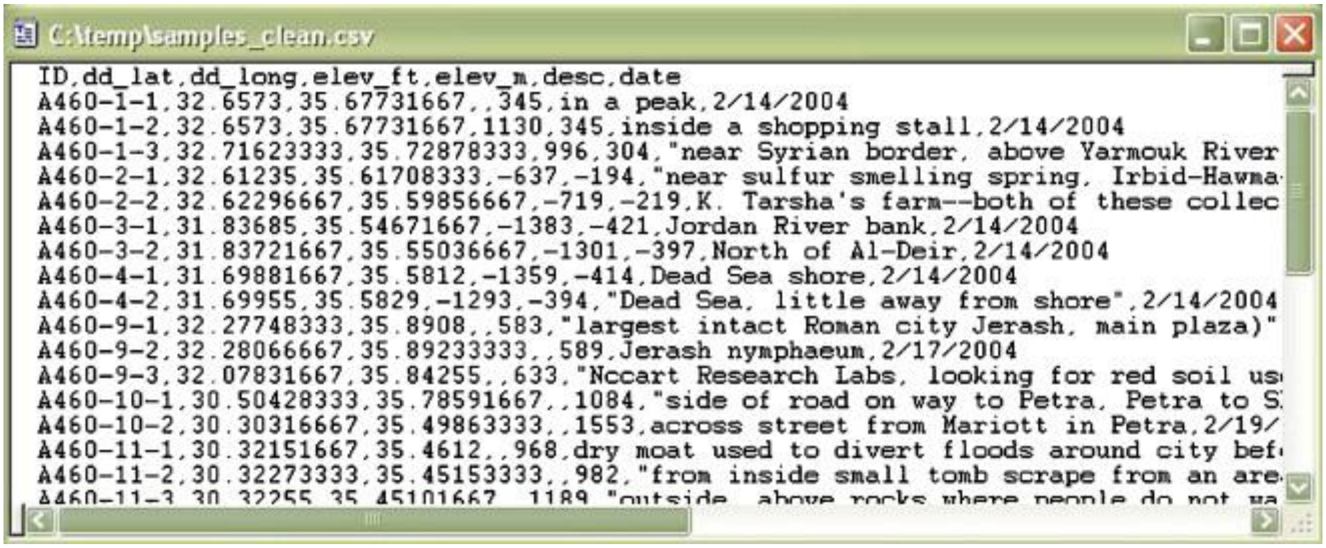
Fig. 2. General overview of the approaches for preparing data files for mapping.

In Approach 1, it was presumed that coordinate data were stored on a GPS device (as waypoints) or in a waypoint management software program. For this, a program called GPSBabel (included in the csv2kml program package) will convert the data directly into a CSV file (explained below). Virtually any GPS-formatted file generated by a GPS device (e.g. Garmin, Magellan, Trimble, and dozens of others) can be converted into a CSV file, and subsequently converted into a KML file, by the csv2kml tool.

Alternatively, it was presumed that coordinate data from a previous project (often termed 'legacy data') were stored either in a simple spreadsheet (e.g. Microsoft Excel; Approach 2) or in a database (e.g. Microsoft Access, Filemaker Pro, SQL Server, Oracle and many others; Approach 3). For these two approaches, the data needs to be saved as a CSV file first (explained below) before conversion into KML by csv2kml. Although the csv2kml tool works on most common desktop computers running Microsoft operating systems, it will only work on MacOS or Linux operating systems when there is a Windows emulator installed.

2.1. The basics of CSV files

The csv2kml tool converts simple comma-separated ascii text files (termed 'comma separated value' or 'CSV' files) into KML format. The CSV input file to be converted into KML is supplied by the user, either from legacy data (Approaches 2 and 3) or from the GPSBabel conversion (Approach 1). Fig. 3 illustrates a simple CSV file. The first line of the file lists the column names separated by commas. Subsequent lines contain the data; each data element is separated by a comma.



C:\temp\samples_clean.csv

```
ID,dd_lat,dd_long,elev_ft,elev_m,desc,date
A460-1-1,32.6573,35.67731667,,345,in a peak,2/14/2004
A460-1-2,32.6573,35.67731667,1130,345,inside a shopping stall,2/14/2004
A460-1-3,32.71623333,35.72878333,996,304,"near Syrian border, above Yarmouk River
A460-2-1,32.61235,35.61708333,-637,-194,"near sulfur smelling spring, Irbid-Hawma
A460-2-2,32.62296667,35.59856667,-719,-219,K. Tarsha's farm--both of these collec
A460-3-1,31.83685,35.54671667,-1383,-421,Jordan River bank,2/14/2004
A460-3-2,31.83721667,35.55036667,-1301,-397,North of Al-Deir,2/14/2004
A460-4-1,31.69881667,35.5812,-1359,-414,Dead Sea shore,2/14/2004
A460-4-2,31.69955,35.5829,-1293,-394,"Dead Sea, little away from shore",2/14/2004
A460-9-1,32.27748333,35.8908,,583,"largest intact Roman city Jerash, main plaza)"
A460-9-2,32.28066667,35.89233333,,589,Jerash nymphaeum,2/17/2004
A460-9-3,32.07831667,35.84255,,633,"Nccart Research Labs, looking for red soil us
A460-10-1,30.50428333,35.78591667,,1084,"side of road on way to Petra, Petra to S
A460-10-2,30.30316667,35.49863333,,1553,across street from Mariott in Petra,2/19/
A460-11-1,30.32151667,35.4612,,968,dry moat used to divert floods around city bef
A460-11-2,30.32273333,35.45153333,,982,"from inside small tomb scrape from an are
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Fig. 3. Example of a CSV file.

2.2. The preparation of CSV files

CSV files can be produced in a number of ways. For example, spreadsheets that were produced in MS Excel format can be saved in the CSV format from within Excel. Database files such as MS ACCESS tables, FoxPro tables or most other databases systems can also produce CSV files in a similar manner. However, in both cases, it is crucial first to make sure the data are formatted properly.

The key to producing appropriate CSV files from an Excel spreadsheet is to remove any extraneous formatting or information (e.g. cell borders and ornamentation, sub-totals, or unformatted text), such that the Excel spreadsheet is a simple columnar list of sample ID codes, locations, and ancillary information (i.e. field observations). Each record (i.e. row) of the spreadsheet should contain information for a single sample, and the first row should contain the names of each field.

How to prepare CSV file properly is best described via an example. Fig. 4 illustrates an improperly formatted Excel file from our own research endeavors in Jordan. The main problems were that both latitude and longitude coordinates were contained in a single field (‘GPS Coordinates’), extraneous formatting symbols were included to describe the coordinates (‘*N*’, the degree symbol, ‘min’, etc.), and the coordinates were not displayed in the Decimal Degrees format.

Sample #	GPS Coordinates	Elevation in Feet	Elevation in meters	Description	Date Collected
A460-1-1	N 32° 39.438 min, E 35° 40.639 min		(+345 m)	in a peak	2/14/2004
A460-1-2	N 32° 39.438 min, E 35° 40.639 min	+1130'	(+345 m)	inside a shopping stall	2/14/2004
A460-1-3	N 32° 42.974 min, E 35° 43.727 min	+996'	(+304 m)	near Syrian border, above Yarmouk River	2/14/2004
A460-2-1	N 32° 36.741 min, E 35° 37.025 min	-637'	(-194 m)	near sulfur smelling spring, Irbid-Hawma-Shuneh	2/14/2004
A460-2-2	N 32° 37.378 min, E 35° 35.914 min	-719'	(-219 m)	K. Tarsha's farm--both of these collections were in Northern part of Jordan Valley	2/14/2004
A460-3-1	N 31° 50.211 min, E 35° 32.803 min	-1383'	(-421 m)	Jordan River bank	2/14/2004
A460-3-2	N 31° 50.233 min, E 35° 33.022 min	-1301'	(-397 m)	North of Al-Deir	2/14/2004
A460-4-1	N 31° 41.929 min, E 35° 34,872 min	-1359'	(-414 m)	Dead Sea shore	2/14/2004
A460-4-2	N 31° 41.973 min, E 35° 34.974 min	-1293'	(-394 m)	Dead Sea, little away from shore	2/14/2004
A460-9-1	N 32° 16.649, E 35° 53.448		583 m	largest intact Roman city Jerash, main plaza)	2/17/2004
A460-9-2	N 32° 16.840, E 35° 53.540		589 m	Jerash nymphaeum	2/17/2004
A460-9-3	N 32°, 04.699 min, E 35° 50.553 min		633 m	Nccart Research Labs, looking for red soil used to treat infection	2/18/2004
A460-10-1	N 30° 30.257 min, E 35° 47.155		1084 m	side of road on way to Petra, Petra to Shoubak, look like lava rock but more dense	2/18/2004

Fig. 4. Example of an improperly formatted excel file. In particular, the GPS coordinates column must be separated into longitude and latitude, removing the N and E designations. Furthermore, the data depicted are in degrees decimal minutes, and they must be converted into decimal degrees.

The reformatted Fig. 4 is depicted in Fig. 5, which is now ready for saving as a CSV file. This is a simple procedure, where one uses 'File->Save As' from the Excel menu, then chooses 'CSV (comma delimited) (*.csv)' as the output file type. For legacy data stored in a database format (e.g. MS Access), one simply needs to reformat the data using the same general principles, and again, save in a CSV format. Once a CSV file has been created, the csv2kml conversion tool is used to specify the name of the file, to name the fields containing the latitude and longitude coordinates, and to convert any other data fields that the user would like to co-display on the map.

ID	dd_lat	dd_long	elev_ft	elev_m	desc	date
A460-1-1	32.6573	35.67731667		345	in a peak	2/14/2004
A460-1-2	32.6573	35.67731667	1130	345	inside a shopping stall	2/14/2004
A460-1-3	32.71623333	35.72878333	996	304	near Syrian border, above Yarmouk River	2/14/2004
A460-2-1	32.61235	35.61708333	-637	-194	near sulfur smelling spring, Irbid-Hawma-Shuneh	2/14/2004
A460-2-2	32.62296667	35.59856667	-719	-219	K. Tarsha's farm--both of these collections were in Northern part of Jordan Valley	2/14/2004
A460-3-1	31.83685	35.54671667	-1383	-421	Jordan River bank	2/14/2004
A460-3-2	31.83721667	35.55036667	-1301	-397	North of Al-Deir	2/14/2004
A460-4-1	31.69881667	35.5812	-1359	-414	Dead Sea shore	2/14/2004
A460-4-2	31.69955	35.5829	-1293	-394	Dead Sea, little away from shore	2/14/2004
A460-9-1	32.27748333	35.8908		583	largest intact Roman city Jerash, main plaza)	2/17/2004
A460-9-2	32.28066667	35.89233333		589	Jerash nymphaeum	2/17/2004
A460-9-3	32.07831667	35.84255		633	Nccart Research Labs, looking for red soil used to treat infection	2/18/2004
A460-10-1	30.50428333	35.78591667		1084	side of road on way to Petra, Petra to Shoubak, look like lava rock but more dense	2/18/2004

Fig. 5. Example of an excel file that has been formatted properly for saving as a CSV file.

Helpful tips that are known to the GIS community but may be unknown to the natural products community include:

(1) Avoid spaces, punctuation, or special characters in header names (e.g. change 'Elevation in Feet' to 'elevation').
(2) Separate coordinates into two fields; one containing longitude (the X coordinate) and the other containing latitude (the Y coordinate).
(3) Remove formatting characters in the coordinates (e.g. remove '*N*', the degree sign, and 'min').
(4) Convert degrees and decimal minutes coordinates or degrees, minutes, seconds coordinates to decimal degrees (explained below).
(5) Latitude coordinates south of the equator (zero degrees latitude) should be preceded by a minus sign. (No plus sign is required for latitude coordinates north of the equator.)
(6) Longitude coordinates west of the Greenwich Meridian (zero degrees longitude) should be preceded by a minus sign. (No plus sign is required for longitude coordinates east of the Greenwich Meridian.)
(7) Remove any blank rows or columns.

Of all the recommendations, conversion into decimal degrees (DD) may seem the most daunting. Web searches using keywords such as 'latitude conversion' will bring up many tools and websites that allow one to convert DMS (degrees minutes seconds) coordinates to DD coordinates. However, most of those sites will only convert one coordinate at a time, and, thus, one may wish to use an operation to convert all the coordinates in a file. One example to convert latitude/longitude coordinates stored in DMS from within a spreadsheet would be to format the coordinate so that each part of the value is separated by a colon, and then multiply the resulting number by 24. For example, a latitude coordinate of 45 degrees, 30 min, and 30 s should be represented initially as 45:30:30. Then, Excel can be used to multiply that number by 24, and the resulting cell should be formatted as 'General'. For the former example, the final answer is 45.508333 decimal degrees. A more formulaic way to represent the conversion is: $\mathrm{DD} = D + M/60 + S/3600$ where DD is decimal degrees, D is degrees, M is minutes, and S is seconds. Alternatively, many common GPS units provide locations in degrees and decimal minutes notation (e.g. 58 degrees, 39.225 decimal minutes or simply, 58 39.225). The formula for converting degrees and decimal minutes to decimal degrees is: $\mathrm{DD} = D + \mathrm{DM}/60$ where D is degrees and DM is decimal minutes. Thus, a degree decimal-minute value of 58 39.225 is entered into the formula as: 58 + 39.225/60 and the result is 58.65375 decimal degrees.

2.3. Installation of the csv2kml conversion and Google Earth programs

The csv2kml conversion program can be downloaded for free from Supplementary materials of the electronic version of this manuscript. Close all open programs, unzip the downloaded file to a new folder, and then execute (i.e. 'double-click') the extracted 'setup.exe' file. The installation program will detect automatically whether or not version 3.5 of Microsoft's .NET framework is installed on the computer. If the proper version of .NET is not installed, the installer will assist in installation of the framework from Microsoft's website. Once the .NET framework is installed, one may be prompted to reboot the computer. Then, check the Windows Start menu for a new item titled 'RTI International,' in which there will be a link to the executable for the main program. If one does not see 'RTI International' in the Windows Start menu, it may be necessary to double-click the setup.exe file again to complete the installation.

The installation package will add a menu item to the Windows Start menu, a quick launch icon to the desktop, and installs a samples folder containing a CSV and a Garmin GPS output file .GDP for a quick testing (typically stored at 'C: Program Files RTI International RTI_csv2kml Samples' if the defaults are used during the install). The Windows Start menu will contain a link to the help documentation in PDF format and a link to the GPSBabel application for advanced users.

Google Earth is freely available for personal use from http://earth.google.com. Google Earth must be installed on the computer to view KML files; if it is not then the view KML file function in csv2kml will attempt to open the KML file in Windows Notepad (showing the KML data as text). To install Google Earth, simply follow the instructions provided by Google.

2.4. Running csv2kml

After installation, the csv2kml program will be accessible from the Windows Start menu. To access it, select 'Start->Program Files->RTI International->RTI_csv2kml'. When the initial screen appears, click 'File->Open' and navigate to a properly formatted CSV file and click 'OK'. When the CSV file is loaded, the csv2kml window shows the contents of the file (Fig. 6). One should examine the data using the left/right and up/down scroll bars to make sure that it is correct. Then, the drop down menus permit selection of the fields containing the '*X* coordinate (longitude)' and '*Y* coordinate (latitude),' respectively. The remaining five dropdown menus are used to select other optional fields in the table that one would like to also see incorporated into Google Earth (e.g. elevation, field observations, bioassay data, and taxonomy). The csv2kml program confirms that the coordinates are in decimal degrees format and that they are within allowable ranges. However, it is up to the user to validate the contents of the input CSV file beyond this. Fig. 7 illustrates an example of a completed file that is prepared for conversion.

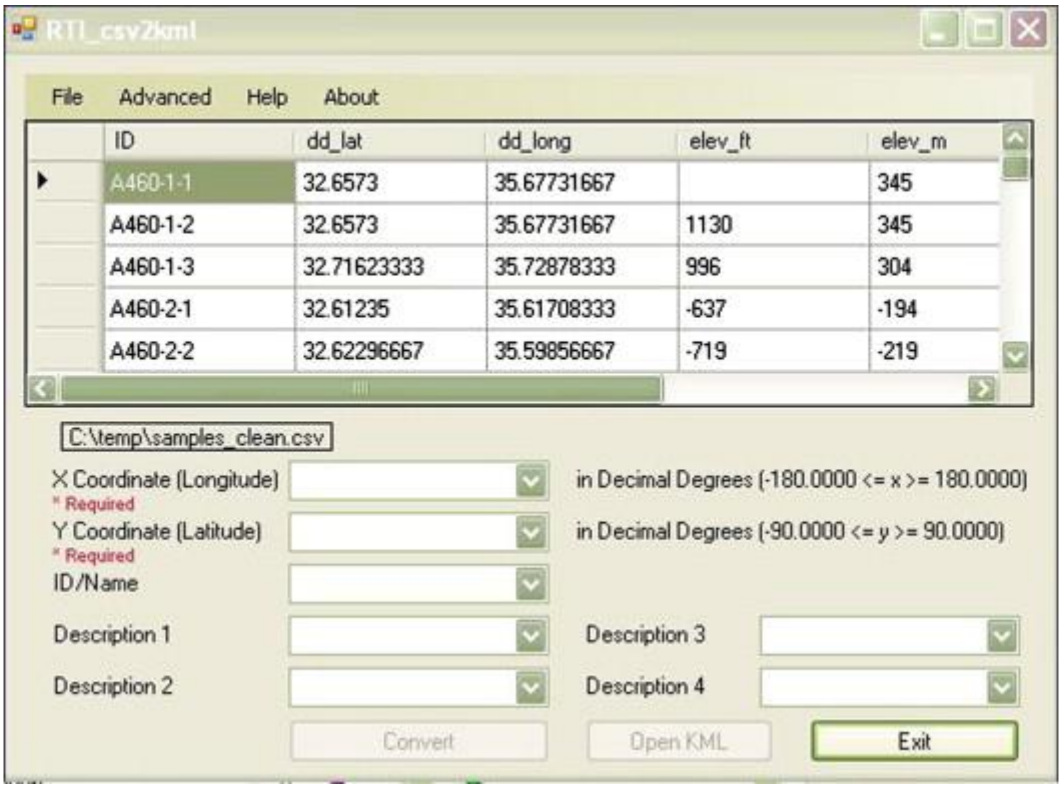

Fig. 6. Example of a CSV file that has been uploaded into the csv2kml conversion program.

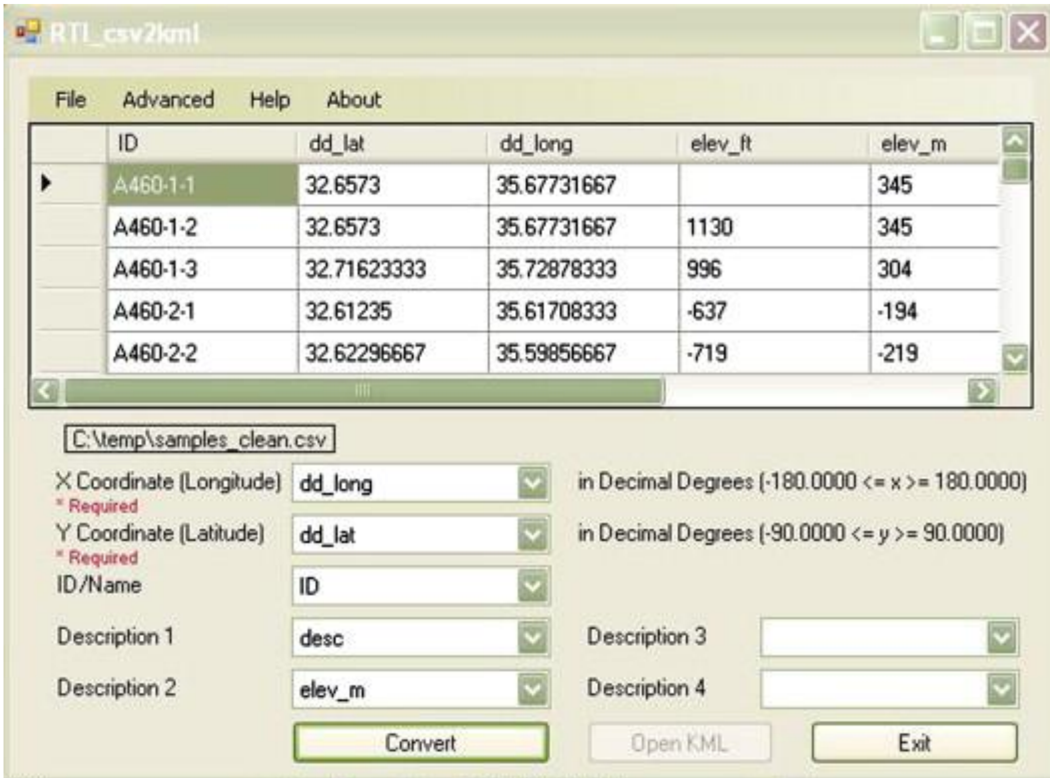

Fig. 7. Example of a CSV file being previewed in csv2kml and how to specify *X* coordinate, *Y* coordinate, ID/Name and description field variables in the conversion.

After filling in the dropdown fields, click the 'Convert' button to start the conversion. If the output file already exists, csv2kml will issue a warning message about overwriting; click 'Yes' to overwrite or 'No' to go back to the csv2kml menu to choose a new file. If one does not want to overwrite an existing file, simply rename the input CSV; the csv2kml application uses the input CSV name and creates a new file by changing the file extension to .kml. If there are any records in the .csv file that don't conform to the comma-separated format, the csv2kml file will issue a warning message and will place the problematic records in an error file that has the same prefix as the conversion file but with the suffix '.err'. Once the conversion is complete, csv2kml issues a message confirming completion and requires one to click 'OK'. From this point, there are two options: (1) opening the converted file in Google Earth directly or (2) exiting the csv2kml program. For the former, simply Click 'Open KML' and Google Earth will open and load the converted kml file. If Google Earth or another KML-associated viewer is not installed, the KML file will open in Windows Notepad (showing the KML data as text).

2.5. Using Google Earth

The following section provides a brief description of how to use Google Earth to view the locations created by the csv2kml file. However, it is beyond the scope of this paper to describe all of the features of Google Earth. Google provides full documentation for Google Earth as well as tutorials and other materials to help users take full advantage of Google Earth (http://earth.google.com).

The sample points in the KML file will appear under the 'My Places->Temporary Places' portion of the table of contents, with each sample point listed therein. Fig. 8 displays the basic Google Earth interface with the sample points displayed on the map and listed on the left side. The mouse can be used to click on any of the KML points in the map to glean information about them. Google Earth will provide the attribute information about the point, and these attributes are the same as the columns specified in the csv2kml interface (Fig. 9). If there are several points within close proximity, the points will expand outward to facilitate selection of a single point.

FIGURES 8 AND 9 ARE OMITTED FROM THIS FORMATTED DOCUMENT

Google Earth's navigation controls in the upper right of the screen can be used to zoom and pan to an area of interest. Alternatively, one can double-click on one of the sample points in the left hand table of contents. Google Earth has many options for creating useful displays. For example, using the Ctrl button while simultaneously dragging the mouse up or down, allows one to tilt and rotate the map to visualize the terrain; this feature was used to generate the images in Fig. 1. To do this, the 'Terrain' check-box located at the bottom of the left-hand table of contents must be checked.

2.6. Converting GPS-formatted coordinate files with GPSBabel

A powerful Open Source GPS conversion tool, termed 'GPSBabel,' is included with csv2kml. GPSBabel can convert virtually any GPS-formatted file into KML or CSV formats. If one uses a GPS unit to collect coordinates (termed 'waypoints'), simply copy the waypoints, routes, or tracks from the GPS unit to the computer using the GPS-provided tools. Then open GPSBabel, select the appropriate file input format and output format to convert it to KML (Fig. 10). If one uses GPSBabel to first convert from a GPS-formatted file to CSV, then it will be possible to convert the resulting CSV file directly to KML using csv2kml. Alternatively, once the CSV file is created, it can be opened in Microsoft Excel or Microsoft Notepad, and fields can be edited and added; csv2kml is then used to create the KML file (per Section 2.4). This may be convenient if, for example, one has new information that should be linked to the coordinates (e.g. taxonomy or bioassay data). GPSBabel can be opened from a link in the Windows Start menu under 'RTI International - > GPSBabel.org' and also from within csv2kml under the 'Advanced' menu item. After the file has been converted, double-click it to open in Google Earth.

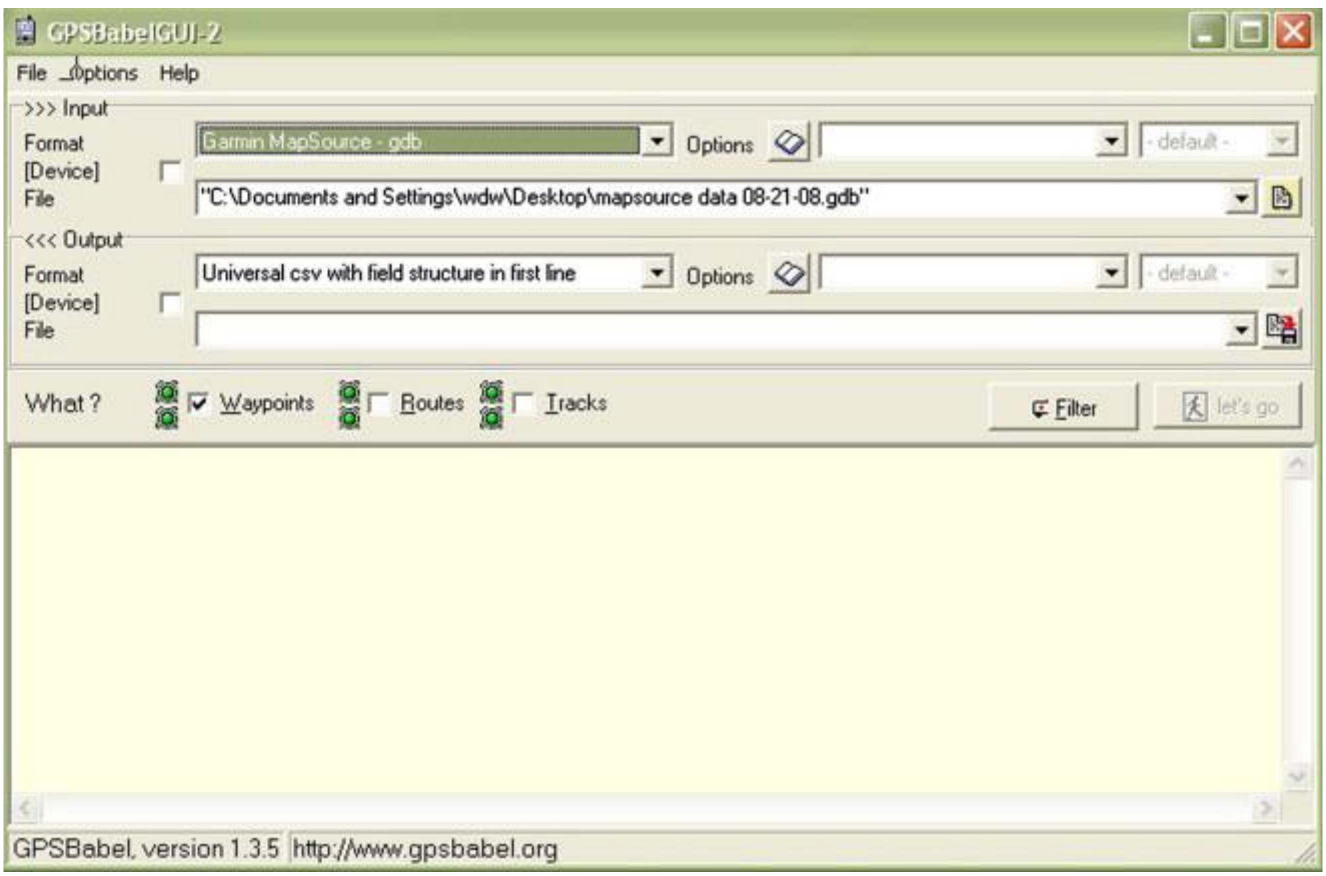

Fig. 10. Example of the GPSBabel conversion tool. GPSBabel allows one to convert from virtually any GPS format to the CSV format.

3. Conclusion

In conclusion, the software described herein facilitates the mapping of collection data by packaging it into a format that is readily useable by Google Earth. Our tool, csv2kml, is open source software, and as such, we welcome additions to it from the research community as new capabilities are conceived and developed. Given the popularity of Google Earth, we anticipate that it will become a mainstay of many personal and research computers; Google most certainly will continue to add new features, such as higher resolution satellite imagery and three-dimensional views. The mapping possibilities are vast, and as such, keeping an open mind and trying many different permutations are probably the best advice we can espouse.

We strongly encourage natural products researchers to embrace the mapping of collections using these types of tools, both for planning purposes, and perhaps more importantly, to communicate these data to other facets of the research community and even the general public. Natural products research begins with nature. All of us know how pollution, population growth, deforestation, and climate change are affecting the natural landscape. How such changes affect natural products research will be determined over time. Being able to visualize the "how, where, and why" questions of natural products research, particularly the tangible aspects of collections and how they relate to the environment, may be a benefit to the entire community. Using rich maps to convey such data graphically helps to break down communication barriers, thereby bringing diverse research ideas together.

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